INVESTIGATION AND QUANTIFICATION OF MONOATOMIC DOPINGS ON BINDING ENERGY OF NANO-SILICON CLUSTERS

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Abstract
Physical and chemical properties of atomic clusters of group-IV elements are receiving a lot of research investigations due to their potential applications in several modern nanotechnological devices. Particular research interest is shown in fundamental and applied aspects of nanosilicon clusters whose properties lie between those of individual atoms and the properties of bulk materials. Therefore, such properties would greatly be affected by the number of atoms, n, constituting these clusters and the binding energy, E_b, between atoms. In this context, we study the variations of E_b as a function of n for small sized clusters ($2 \leq n \leq 20$ at) of intrinsic nano-Si as well as monoatomic doping effects with (i) transition metals: Ag, Au, Co, Cu, Fe, Mn, Ni, Ti, (ii) rare earth: Eu, Gd, La, Lu, Tb, (iii) non metals: C, P & (iv) alkali metals: Na. To do so, we selected the most widely reported computing methods: (a) Hartree-Fock (HF) and Post HF, (b) Density functional theory (DFT) with Local Density Approximation (LDA), Generalized Gradient Approximation (GGA) and functional hybrids. Finally, the results are quantified semi-empirically in order to deduce relations between binding energy and cluster sizes for different doping elements. The obtained curves of E_b versus n_{Si} showed similar behaviors for all dopants and with various methods; these curves can be divided into three regions: an initial sharp increase ($2 \leq n \leq 5$ at), followed by a transition region ($5 \leq n \leq 10$ at) and ending by a saturation region (n>10 at). A close analysis of regions I and II, i.e., for ($2 \leq n \leq 10$ at) led to the following observations: (i) similar variations (E_b increases with n), but not sensitive to the choice of neither the dopant nor the method, (ii) the variation of E_b versus n takes an exponential form whose quantification was found to be of the form: $E_b = C + \alpha \exp(-n_{Si}/\beta)$ with C, α and β being characteristic constants which we deduced for each method and its variants (iii)similar variationfordoped nano-Si clusterscalculatedbythe same method: the increase inatomic radius, R_{at}, of thedopant atomcauses adecrease in$E_b$and (iv) the E_b for doped nano-Si clusters put into evidence the great effect of the doping element. This effect may provide a useful way of controlling the binding energy by choosing an impurity atom to dope Si clusters.Moreover, the importance of the above deduced formulas lies not only in their applicability to all dopants and methods but also in the possibility of predicting binding energies for known atom numbers in clusters and vice versa.

Keywords: *Doping, Nanosilicon, Clusters, Binding energy.*